

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 33.7

Global applicability domain: Inside

Local applicability domain index: 4.56e-01

Confidence level: 6.05e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isoamyl ether</div> <div>Measured: 170</div> <div>Predicted: 137</div>	<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 219</div> <div>Predicted: 151</div>	<div>Image not found</div> <div>DEET</div> <div>Measured: 2.40</div> <div>Predicted: 4.09</div>
<div>Image not found</div> <div>Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>(1R,2S,5R)-(-)-Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>Isoprothiolane</div> <div>Measured: 37.2</div> <div>Predicted: 28.5</div>